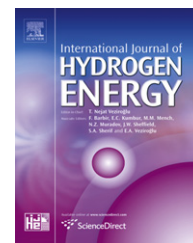


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# Simulation on thermoelectric device with hydrogen catalytic combustion

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## ABSTRACT

The micro-thermoelectric-generator based on catalytic combustion of hydrogen and oxygen was designed. With the application of general finite reaction rate model in CFD software of FLUENT, the effect of inlet parameters on the highest temperature difference between the hot and cold plate of the generator was studied. Results showed that, the temperature in the heating and cooling channel of the micro-thermoelectric-generator was uniform; with the increasing of inlet reactant temperature, the highest temperature difference increased, but the total efficiency of the generator decreased. Results can be used to the further design and optimization of micro-thermoelectric-generator based on hydrogen catalytic combustion.

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## 1. Introduction

Thermoelectricity is an effective way which can be used to take full advantage of waste heat, solar energy and geothermal energy to generate electric power. As a special power producer, it has the advantage of simple piping, sturdy and durable, no moving parts and noise [1–3]. However, the adopting of the above energy such as using solar as the thermal source for thermoelectric generator is inconvenient, because its energy density is very low, and sometimes it relies on the time and season. As a result, it is unfavorable to be taken as a heat source for a portable power generator. Through the application of fossil fuels such as hydrocarbon fuels can overcome the above disadvantage of thermoelectric generator, but it still has the harmful results of CO<sub>2</sub> emission, high temperature and therefore still unfavorable for portable usage [4–6]. So in this paper, the novel micro-thermoelectric-generator based on hydrogen catalytic combustion was designed and simulated. Through

the usage of heat from hydrogen catalytic combustion, not only zero emission of CO<sub>2</sub> can be achieved, but also temperature of the generator is reduced due to flameless catalytic combustion of hydrogen [7–9]. Therefore it is safe and portable. The cold side of the thermoelectric module can be cooled by the incoming flow of the hydrogen and oxygen reactants with atmospheric temperature. The effects of inlet parameters on the thermoelectric generator temperature difference were studied and the temperature distribution in the channel was also discussed to find the maximum temperature difference between hot and cold side of the module.

## 2. Physical, mathematical and kinetic model

The physical model used by simulation was shown in Fig. 1. It includes the reactants flowing channel, one thermoelectric module, corresponding cold and hot side material, thermal

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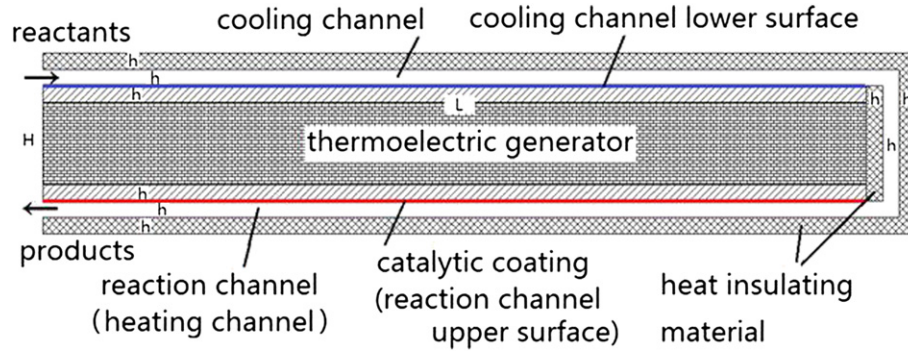


Fig. 1 – Thermoelectric generator physical model which is based on hydrogen catalytic combustion.

isolation material and the hydrogen catalytic combustion coating.

Reactants flow into the generator from the inlet through the cold side channel, and then changes direction to the outlet in the hot side channel at which hydrogen catalytic combustion reaction takes place. Heat is generated on the catalytic surface and conducts to the thermoelectric cold side through the body of the generator. Therefore, temperature difference is generated between the hot and cold side of the thermoelectric module as well as power. The length  $L$  and height  $H$  of the thermoelectric module is 40 mm and 5 mm respectively. The thickness  $h$  of the other materials and flowing channel are all 1 mm.

Mathematical model of the reaction channel in the generator was established based on the following assumptions. Only the catalytic surface reaction of hydrogen combustion with oxygen was considered; the boundary of outer surface was thermal isolation; reaction occurred in a steady state and a plug flow was assumed, so there was no back mixing phenomenon in the flowing channel; radiation heat transfer and body force were neglected; properties such as density, molecular viscosity and thermal conductivity were calculated assuming an ideal gas mixture. With the application of general finite reaction rate model in CFD software of FLUENT, the governing equations for analysis of the reacting flow in the heating fluid side channel of the generator were shown in the following.

Mass balance:

$$\frac{\partial(\rho V_j)}{\partial x_j} = 0 \quad (1)$$

Species balance:

$$\rho V_j \frac{\partial Y_s}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial Y_s}{\partial x_j} \right) + R_s \quad (2)$$

Momentum balance:

$$\frac{\partial(\rho V_j V_i)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i} \right) \right] \quad (3)$$

Energy balance:

$$-\frac{\partial}{\partial x_j} \left( \lambda \frac{\partial}{\partial x_j} \right) = \frac{\partial}{\partial x_j} \left( \sum \rho D \frac{\partial Y_s}{\partial x_j} h_s \right) + q \quad (4)$$

Ideal gas law:

$$p = \rho RT \sum \frac{Y_s}{M_s} \quad (5)$$

At present, there are studies of hydrogen catalytic combustion adopting mechanism of heterogeneous reaction kinetics coming from CHEMKIN software database [10,11], and there are also researches which use the total reaction kinetics [12,13]. In this paper, the main purpose was to analyze the effect of inlet parameters such as velocity on temperature difference at both side of the generator, so the simple single rate equation of hydrogen catalytic combustion kinetics was adopted as shown in equations (6) and (7). And furthermore the kinetic model was tested and compared with mechanism model results in reference [12].



$$r = A C_{\text{H}_2} C_{\text{O}_2} \exp(E/RT) \quad (7)$$

In the above equations,  $Y_s$ ,  $M_s$ ,  $R_s$  are the mass mole fraction, mole weight and consumption rate of species  $s$  which refers to  $\text{H}_2$  and  $\text{O}_2$  respectively.  $h$  is the enthalpy of the mixture;  $q$  is heat of reaction;  $D$  is the diffusion coefficient of mixture;  $\lambda$  is the conductivity;  $\mu$  is coefficient of viscosity; and  $\rho$  is density of mixture. The conductivity of the thermoelectric material in this paper comes from reference [14].  $r$  is reaction rate of hydrogen catalytic combustion,  $A$  is the exponential factor of the rate,  $C_s$  is the mole concentration of the species  $\text{H}_2$  and  $\text{O}_2$  and  $E$  is the active energy of the reaction. Since the highest combustion efficiency and the higher surface temperature can be obtained at the hydrogen oxygen equivalence ratio of 1 [15], the hydrogen oxygen equivalence ratio of 0.125:0.875 was adopted.

### 3. Results and discussion

In simulation, through variation of the inlet parameters such as reactants inlet velocities of  $V_{\text{in}}$  and the inlet temperatures of  $T_{\text{in}}$ , the maximum temperature difference between the cold and hot sides of the thermoelectric generator  $\Delta T$  was studied.

Firstly, at reactants inlet velocity of 0.2 m/s and inlet temperature of 1000 K, the kinetic model testing and verification was carried out as shown in Fig. 2 by comparing the results of detail mechanism model including 13 surface reactions in reference [12] and single rate equations. Results indicated that the maximum temperature difference results with detail mechanism between thermoelectric generator

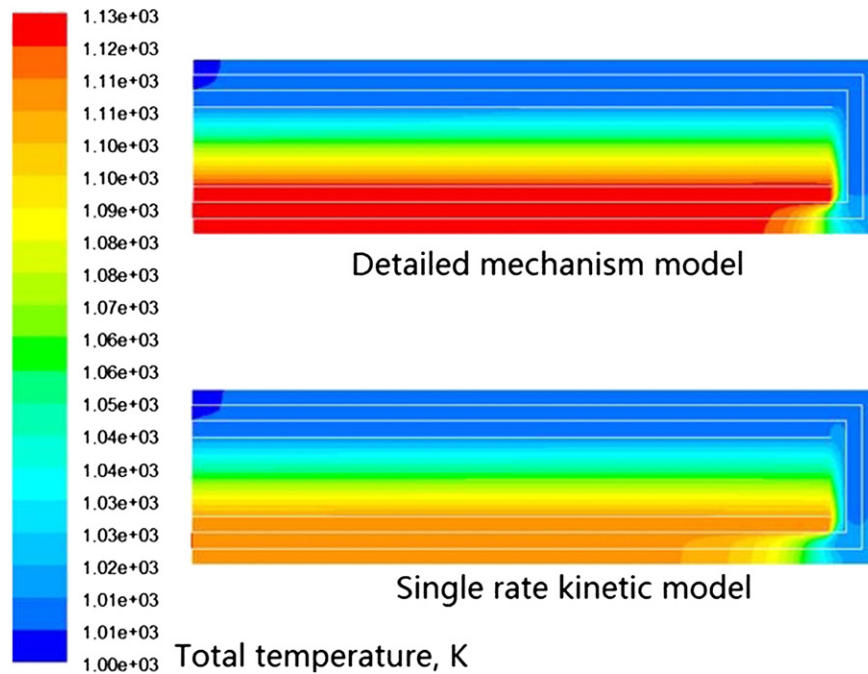


Fig. 2 – Comparison of temperature distribution in the generator with detail mechanism and single rate kinetic model.

cold and hot sides were 30 K greater than the single rate model used in this paper. The main reason was that all one rate models cannot account for the heterogeneous induced radical inhibition and yielded no homogeneous ignition. But the error was only about 3% when taking the inlet temperature as reference. What is more, the temperature distribution was very similar for both situations. So the single rate kinetics of hydrogen oxygen catalytic combustion model was adopted.

In the same conditions, the output power of thermoelectric generator is in proportion to the temperature difference between the cold and hot sides. Therefore, the effect of inlet parameter on maximum temperature difference  $\Delta T$  was studied as shown in Fig. 3. Maximum temperature difference

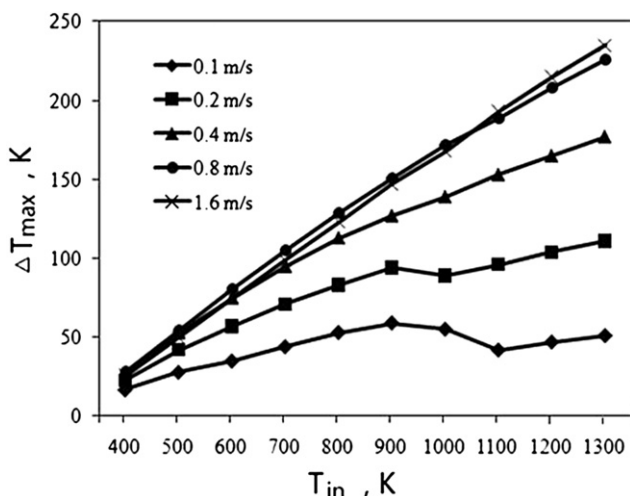


Fig. 3 – The maximum temperature difference  $\Delta T$  at different inlet temperature and inlet velocity.

$\Delta T$  of the generator increased with inlet temperature at all different inlet velocities. With increasing of inlet temperature, catalytic combustion reaction rate of hydrogen increased, therefore, at the same reactants flow rate, hydrogen conversion raised and this resulted in generated heat of reaction increased. This heat finally conducted to the cold side of the generator and led to the temperature difference increasing. However, as the velocity increasing, the total reactant flowing into the reaction channel increased, therefore, at the same time, the generation of reaction heat increased, which also led to the increasing of  $\Delta T$ . However, when inlet velocity increased to certain degree, increase of  $\Delta T$  became relatively small, and at certain temperatures, it decreased with inlet velocity. Since residence time of the reactant in the reaction channel reduced, some portion of the reactant flowed out of the generator without reaction, so the generation of heat

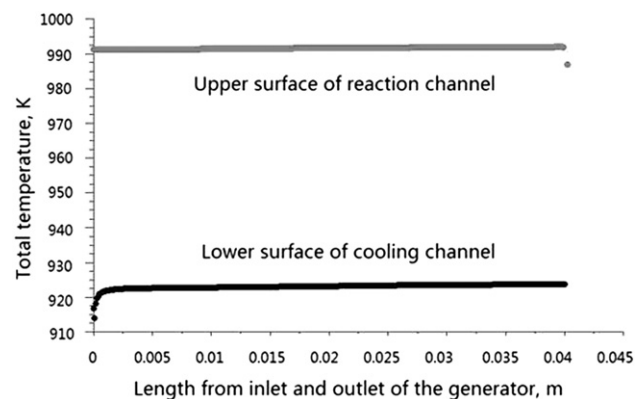


Fig. 4 – Temperature distribution on cold and hot sides of the generator at condition of  $T_{in} = 900$  K and  $V_{in} = 0.2$  m/s.

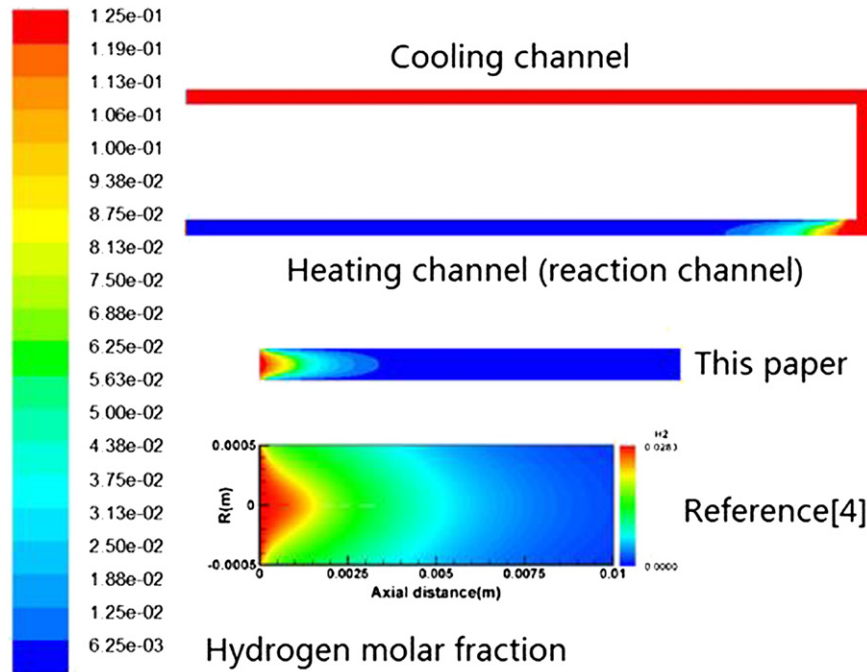


Fig. 5 – Hydrogen molar fraction at  $T_{in} = 900$  K and  $V_{in} = 0.2$  m/s.

reduced and thereupon  $\Delta T$  decreased. When the temperature exceeded 1000 K, combustion rate enhanced greatly, so  $\Delta T$  increased again although reactant flow rate increased dramatically. In addition, at relatively lower inlet velocities (0.1 m/s, 0.2 m/s),  $\Delta T$  of the generator showed a variation of increasing firstly then decreasing with the inlet temperature. This indicated that at the temperature of about 900 K, diffusion limitation occurred for reactants of hydrogen and oxygen spreading from the channel center to the catalytic surface. However, with the elevating of temperature, this limitation gradually vanished, so  $\Delta T$  of the generator again raised.

In the conditions of  $T_{in} = 900$  K,  $V_{in} = 0.2$  m/s, temperature distribution on the upper surface of reaction channel (hot side) and lower surface of the cooling channel (cold side) was shown in Fig. 4. It can be seen that hydrogen and oxygen reacted on the catalytic surface immediately, and the heat released by catalytic combustion reaction raised the temperature of the reaction channel. The highest temperature was 995 K, along with the flow direction it decreased slightly. At the same time, temperature on the cold side was raised from 900 K to 922 K and increased gradually. Generally speaking, temperature difference between cold and hot sides of the generator was approximately uniform in all considered conditions, this indicated that the adoption of hydrogen combustion as thermal source and inlet reactants as cooling medium of the generator is reasonable. Along both cold and hot sides, temperature variation is very small because there was no back mixing phenomenon in the flowing channel, the main temperature difference came from the heat transfer between cold and hot sides. The single point in the hot side temperature distribution was due to heat conduction between the main combustion steam and the catalytic coating/heat insulating materials, which resulted in a much lower temperature in

local. The temperature at the start of the reaction channel seems to experience a discontinuity from this point to the maximum temperature of 995 K. Because temperature on the heat insulating material outer wall which connects cooling channel lower surface and reaction channel upper surface was not shown in Fig. 4.

Molar fraction distribution of hydrogen in reaction channel in condition of  $T_{in} = 900$  K,  $V_{in} = 0.2$  m/s was shown in Fig. 5. For comparison, hydrogen molar fraction in the reaction channel with single rate model in this paper and detailed mechanism model in reference [11] was analyzed. Results showed that hydrogen catalytic combusted intensively with

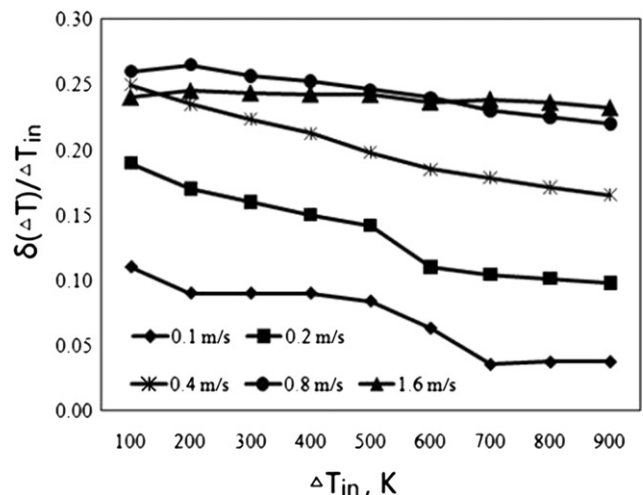


Fig. 6 – Changes of increment of maximum temperature difference with inlet temperature increment.

oxygen at the inlet of the heating channel and converted almost completely near the inlet of reaction channel. This distribution of hydrogen molar fraction matched with the temperature distribution. Conversion of hydrogen was almost 100%. Both distribution in this paper and reference was very similar as could be seen in Fig. 5.

Although the maximum temperature difference of the generator increased with inlet temperature as analyzed above, with the increasing of inlet temperature, requirement for the thermoelectric material also increased. In addition, outlet of temperature of the generator was also high, and this led to waste of fuel energy. Actually, as could be seen in Fig. 6, when plotting the increment of maximum temperature difference  $\delta(\Delta T)$  ( $\Delta T - \Delta T_{400\text{ K}}$ ) with inlet temperature increment  $\Delta T_{\text{in}}(T_{\text{in}} - 400\text{ K})$ , it indicated that  $\delta(\Delta T)$  decreases with increasing of  $\Delta T_{\text{in}}$ . As efficiency of the generator is in proportion to the temperature difference  $\Delta T$ , this decrement of  $\delta(\Delta T)$  showed that total efficiency of the generator decreased with inlet temperature.

#### 4. Conclusions

The adoption of hydrogen catalytic combustion as a thermal source for thermoelectric generator is an efficient way to improve its portability and energy density. It can also reduce greenhouse gases emission. In this paper, a novel thermoelectric generator was designed and analyzed with hydrogen catalytic combustion as a thermal source and lower temperature inlet reactants as a cooling medium. Results showed that temperature distribution in the heating and cooling channel was approximately uniform, which could receive a better power output for the generator. The conversion of hydrogen was almost complete, indicating that it was reasonable to improve energy density by increase inlet hydrogen flow. Although increase of inlet reactant temperature can improve maximum temperature difference between cold and hot sides of the generator, it is better to adopt lower inlet temperatures in order to receive higher total efficiency of the generator. The results can be used as a reference for further study and optimization of thermoelectric generator based on hydrogen catalytic combustion.

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